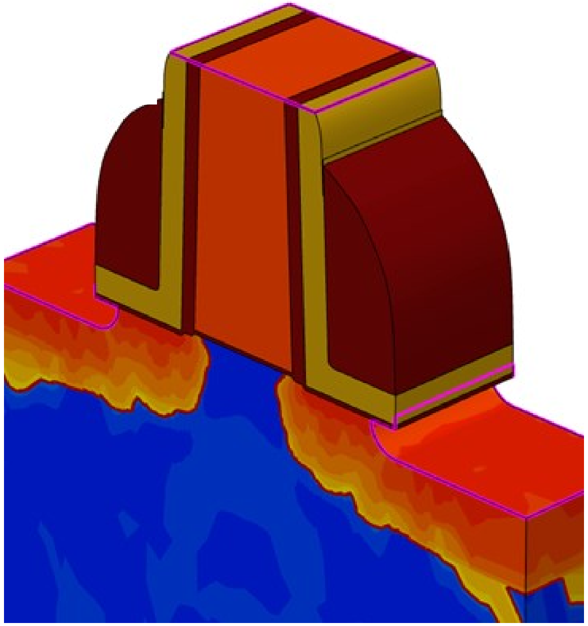
Technology Computer Aided Design (TCAD) Laboratory

Lecture 3, Overview of Synopsys Sentaurus TCAD



[Source: Synopsys]

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University of Bologna, Italy

Outline

- Sentaurus Tools
- TCAD simulation flow
- Starting TCAD: Sentaurus Workbench
- Sentaurus Structure Editor
- Sentaurus Device
- Output examples
- Conclusion

Outline

✓ ***Sentaurus Tools***

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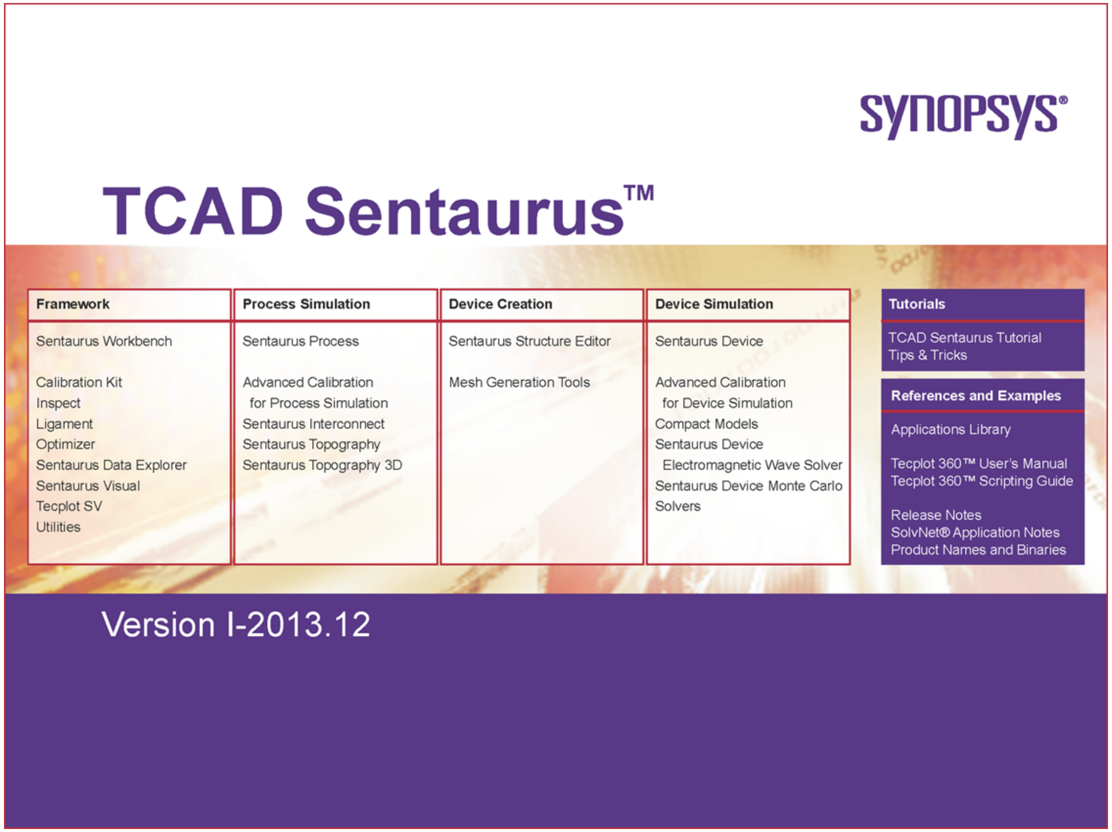
Synopsys TCAD Sentaurus tools

- Synopsys TCAD Sentaurus is a **software suite** made by several tools (each one with its own programming language)
- The starting page of the **Synopsys TCAD manual** contains the link to the manual of each tool



SYNOPSYS®

TCAD Sentaurus™

Framework

Sentaurus Workbench

Calibration Kit
Inspect
Ligament
Optimizer
Sentaurus Data Explorer
Sentaurus Visual
Tecplot SV
Utilities

Process Simulation

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Advanced Calibration
for Process Simulation
Sentaurus Interconnect
Sentaurus Topography
Sentaurus Topography 3D

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Sentaurus Structure Editor

Mesh Generation Tools

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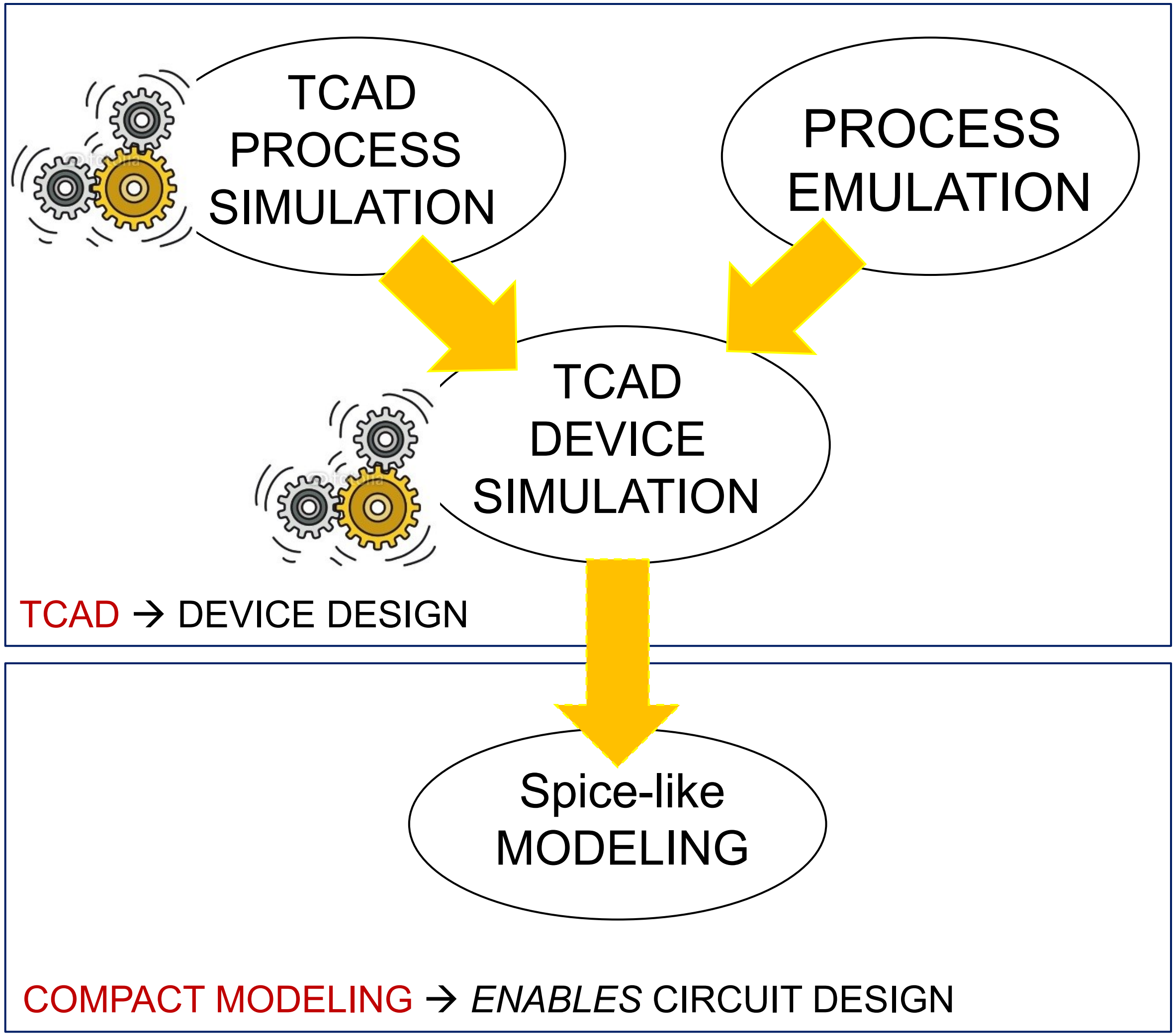
Modeling of semiconductor devices: typical flow



TCAD PROCESS SIMULATION

PROCESS EMULATION

TCAD DEVICE SIMULATION

TCAD → DEVICE DESIGN

Spice-like MODELING

COMPACT MODELING → *ENABLES* CIRCUIT DESIGN

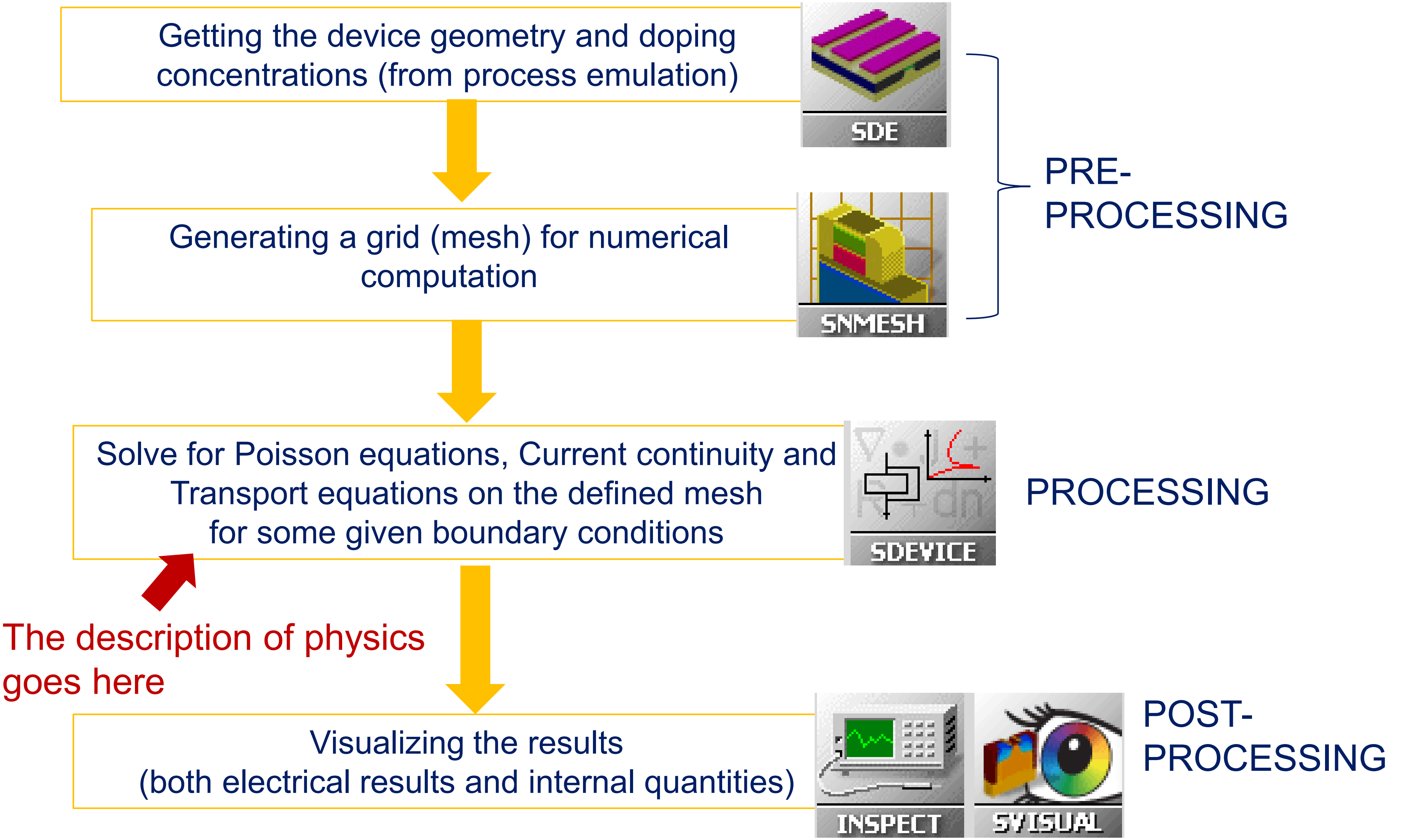
Process Emulation.

Process steps are not simulated but emulated, i.e. the device structure is realized through **somewhat idealized procedures that mimic real process flow.** Process emulation is used for first order device analysis (e.g. targeting a device for new specs., exploring new device concepts). Process simulations can be done once a new device architecture has been optimized by means of device simulation in order to (a) investigate process non-idealities, (b) target process specs.

Compact Modeling.

Compact modeling is a methodology strictly related to TCAD. Once the physics of the device has been verified by TCAD, the device electrical characteristics can be "synthesized" by **analytical functions** that can be physically-based or simply behavioral. Compact modeling is needed to provide the **"device model cards"** to the circuit designers for circuit simulations.

Going through the DEVICE SIMULATION steps



Getting the device geometry and doping concentrations (from process emulation)

Generating a grid (mesh) for numerical computation

PRE-PROCESSING

Solve for Poisson equations, Current continuity and Transport equations on the defined mesh for some given boundary conditions

PROCESSING

The description of physics goes here

Visualizing the results (both electrical results and internal quantities)

POST-PROCESSING

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Loading TCAD environment in the lab (1)

Open Sentaurus Workbench (SWB)

1. Connect Ethernet cable
2. Turn-on the laptop
3. insert username and password
4. type `startx`
5. press `Alt-P ;` type `terminology`
6. Connect to ARCES machine “bue” `ssh –Y bue`
7. Loading the environment variables `source .ISErc`
8. type `swb & ;` click on swb window `;` press `Alt-Shift-2 ;` press `Alt-2`

Open Sentaurus manual:

1. Press `Alt-3 ;` press `Alt-P;` type `terminology`
2. type `evince TCAD/front.pdf & ;` press `Alt-Shift-4`

Useful shortcuts & commands:

Select a desktop: `Alt-`*number*

Resize window: `Alt-`*dx touchpad button*

Move window: `Alt-`*sx touchpad button*

Get control to a terminal where some program has ben launched `CTRL-C`

Close a remote connection: `logout`

Close startx: `Alt-Shift-Q`

Back to login page: `CTRL-D`

Power off the pc: `Alt-Shift-Q ; poweroff`

N.B. Italian keyboard: ~ : alt gr + ì   { }: alt gr + ↑ + [ ]   _: ↑ -

Loading the TCAD environment in the lab (2)

A few words on `source .ISErc`

.ISErc is a **configuration file** stored in the home directory which contains some useful commands and settings:among the others, tells OS where finding out TCAD software installation and executables, tells OS how to get the license file and where user’s SWB projects reside. In addition, it contains:

```
setenv OMP_NUM_THREADS 4
setenv NCPUS 4
```

max number of simultaneous threads

max number of CPUs used simultaneously

code parallelization

```
# .exe
alias swb "/sw/CAD/TCAD/I_2013.12/bin/swb"
```

Set gedit as default editor

on swb window

`F12`

scroll down to editor and click on the ⊞ symbol

select `text`

click inside the bar at the top and type `/usr/bin/gedit`

Sentaurus Workbench: general information

- It is the main tool **interface** which can be Windows-like controlled
- From Sentaurus Workbench (SWB) all the **simulation flow** can be controlled
- Simulations trees with variation of parameters in a **matrix organization** can be created
- An instance in the SWB tool is called “**Project**”
- When a project is saved, a directory is created. ASCII files containing the details of the saved project are created in the directory (in particular the `gtree.dat` file contains the details of the simulation tree)
- Essential vocabulary to understand SWB operations:
  - **Scenario**= to simplify the visualization, the whole simulation tree (the whole project) can be divided in more than one scenario (it means that one project can be divided in more trees)
  - **Tool**= one of the Sentaurus TCAD tools (e.g. sde, sdevice, inspect, etc.).
  - **Parameter**= a variable (it can be a dimension, a physical property, a logic flag..)
  - **Experiment**= a row in the simulation matrix
  - **Node**= a point of the simulation matrix. Each point of the matrix is a “node”.
    - Real node: node that can be executed (one for each tool). They are colored according to the execution status of the corresponding simulation job
    - Virtual node: node that cannot be executed
  - **Root**= part of a row (i.e. of an experiment), from a given node to the left
  - **Leave**= part of a row (i.e. of an experiment), from a given node to the right

Sentaurus Workbench: configuration and shortcuts

`Project` → `New` → `Project` → `Configuration` → `Research`

`Research` provides maximum flexibility, while `Standard` provides maximum level of consistency

`Edit` → `User Preferences` →

`Default View Options` → `Show Pruned` → `false`

To prune a node means to cancel an experiment from the simulation tree

`Scheduler` → `Local jobs` → `Maximum number of simultaneous jobs` → `10`

The scheduler is the software tools which organizes the execution of the simulations

`Scheduler` → `Local jobs` → `Default Nice Level` → `1`

The lower the `Default Nice Level` (1 is the minimum value) the higher the priority by which the simulation is running by the operating systems

`F5` refresh

`CTRL-P` node preprocessing ; `CTRL-R`: node running ; `CTRL-T` abort node execution

`F6` edit parameter value in a node

`F6` node explorer

`F9` show/hide node number

Sentaurus Workbench: useful commands

`Project → Operations → Unlock`

Unlock project blocking (sometimes the software prevents project modifications (block) and you need to unblock this protection to further modify the project itself)

`Parameter → Add`

Add parameters

`Experiments → Create Default Experiments`

To start a new trees: it creates the root experiment with default values parameters

`Experiments → Add New Experiment`

To add a new experiment

`[select a node] → Nodes → Extend Selection to Experiment → Experiments → Add Values`

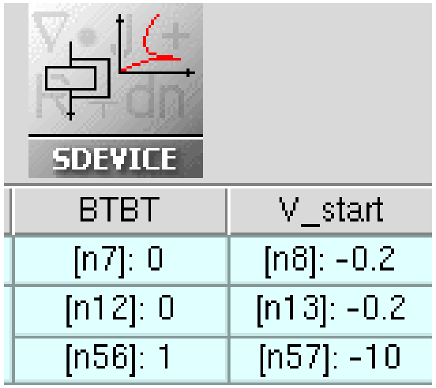
To branch the trees by adding values to a selected experiment only

`[select a node] → Nodes → Extend Selection to Leaves → Nodes → Prune`

To cancel a branch in the experiment tree

Sentaurus Workbench: use of `@`

To use parameters, those must be placed between a pair of `@` in the tools command files (see later). Example: for the BTBT (Band-to-Band-Tunneling physical model) flag to be an Sdevice variable, in the Sdevice command file BTBT must be indicated as `@BTBT@`



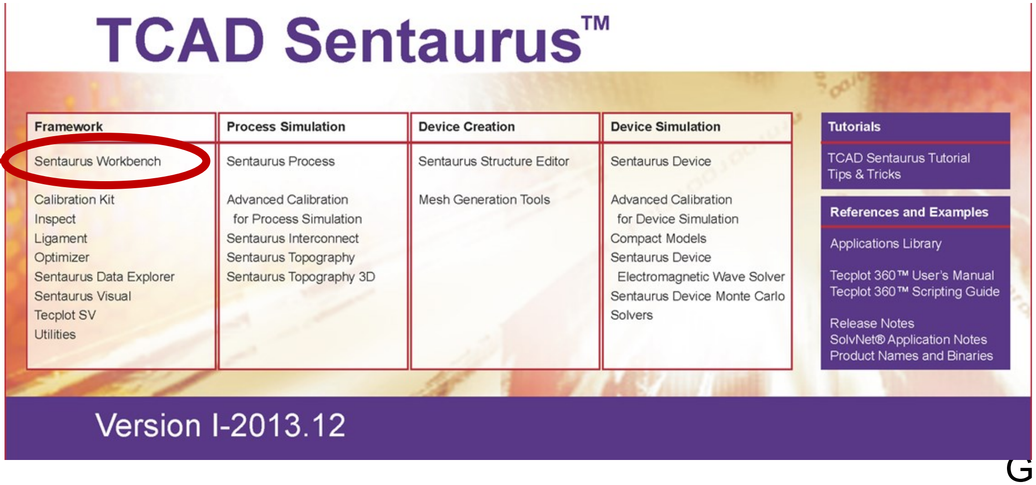
SDEVICE

BTBT	V_start
[n7]: 0	[n8]: -0.2
[n12]: 0	[n13]: -0.2
[n56]: 1	[n57]: -10

The pre-processing steps basically writes how many files how many are the project's experiments, in each of them substituting the `@BTBT@` with the value of BTBT in the node corresponding to the given experiment.

Therefore, a **pre-processing** step is mandatory before an execution of a simulation

- Although we have thoroughly review the most important feature, many **other functionalit**ies are available in SWB (to name a few: include Tcl code blocks, cut & paste scenario's blocks, conformity checks): always refer to the user guide embedded in the manual front-page.



TCAD Sentaurus™

Framework	Process Simulation	Device Creation	Device Simulation
Sentaurus Workbench	Sentaurus Process	Sentaurus Structure Editor	Sentaurus Device
Calibration Kit Inspect Ligament Optimizer Sentaurus Data Explorer Sentaurus Visual Tecplot SV Utilities	Advanced Calibration for Process Simulation Sentaurus Interconnect Sentaurus Topography Sentaurus Topography 3D	Mesh Generation Tools	Advanced Calibration for Device Simulation Compact Models Sentaurus Device Electromagnetic Wave Solver Sentaurus Device Monte Carlo Solvers

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Sentaurus Structure Editor

- Tool that can be used for process *emulation*
- It allows defining
  - device materials & geometry (1D,2D,3D)
  - doping
  - contacts

N.B. 3D TCAD simulations are available in Sentaurus and much used especially by industry (need of precise results on particular application in which the device process/geometry is usually well known). On the other hand we will deal only with 2D simulations, for the sake of simplicity

- Within Sentaurus Structure Editor (SDE), the meshing operation must also be performed
- Better to use it in **batch mode** to increase program flexibility and power
- Input file where to write SDE command in text form must be named `sde_dvs.cmd`
- Once SDE is run, two files are produced:

n*nodenumber*_bnd.tdr for the visualization of the produced device geometry

n*nodenumber*_msh.tdr to visualize the device geometry & the numerical mesh

- The difficult part about SDE is of course not programming in itself, but understanding and evaluating the simplification inherent to the idealized geometry drawings !
- Also the choice of the numerical mesh is sometimes not at all trivial (critical for the convergence of the numerical algorithm)

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Sentaurus Device

- Tool that defines the partial differential equations to be solved, i.e. **it defines the physical model** (e.g. the drift-diffusion model, which consists in the Poisson equations and the current continuity equations)
- **Boundary conditions** (typically bias at the electrodes) must also be defined
- The **material parameters** of the physical model employed must be provided in a separate file
- It is possible to perform **sweeps of the boundary conditions** in order to get device electrical characteristics
- Also **parameters for the numerical solvers** implemented in the software must be defined
- Input files:

  `sdevice_des.cmd` for physical models, boundary conditions and numerical parameters

  `sdevice.par` to enter the model material parameters

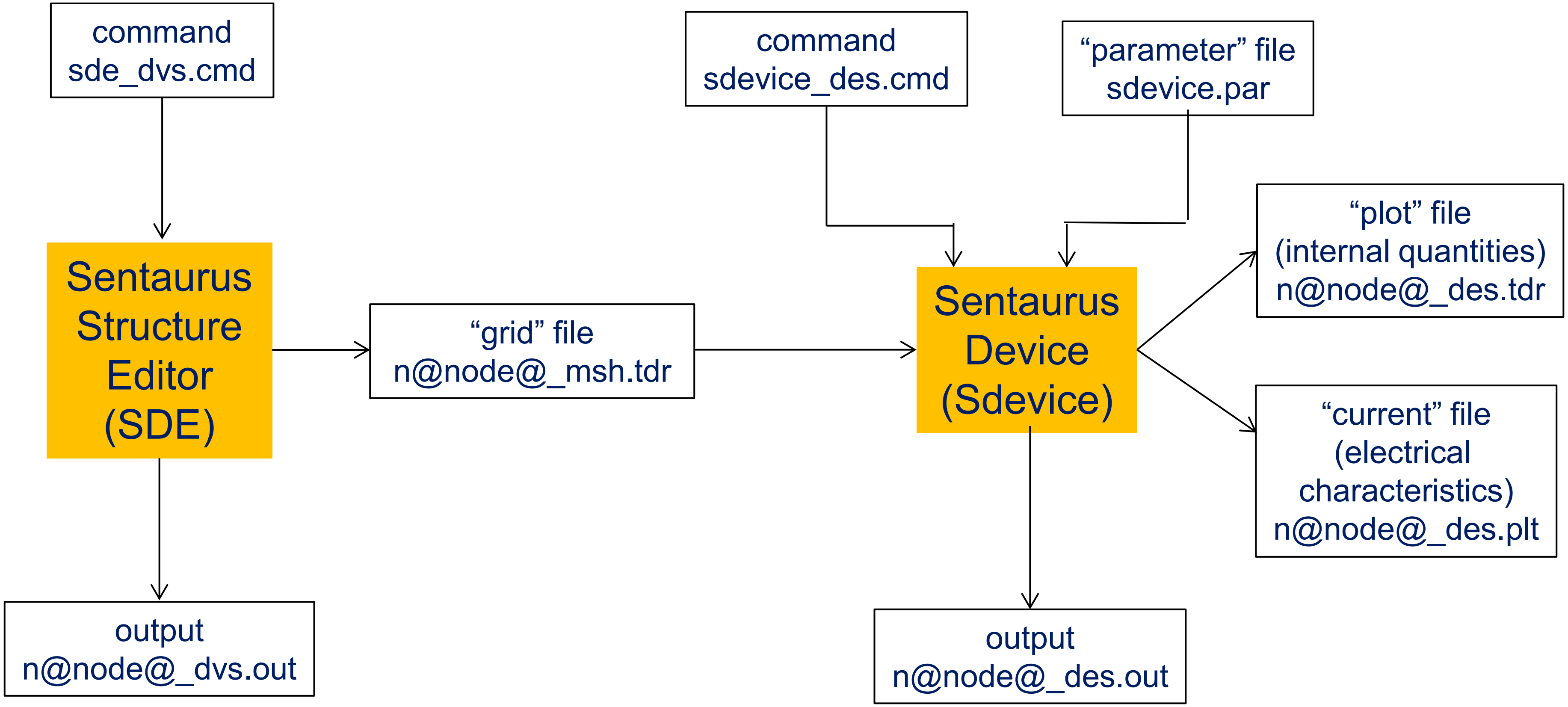
- Output files:

  n*nodenumber*_des.tdr for the visualization of the simulated physical quantities on the domain

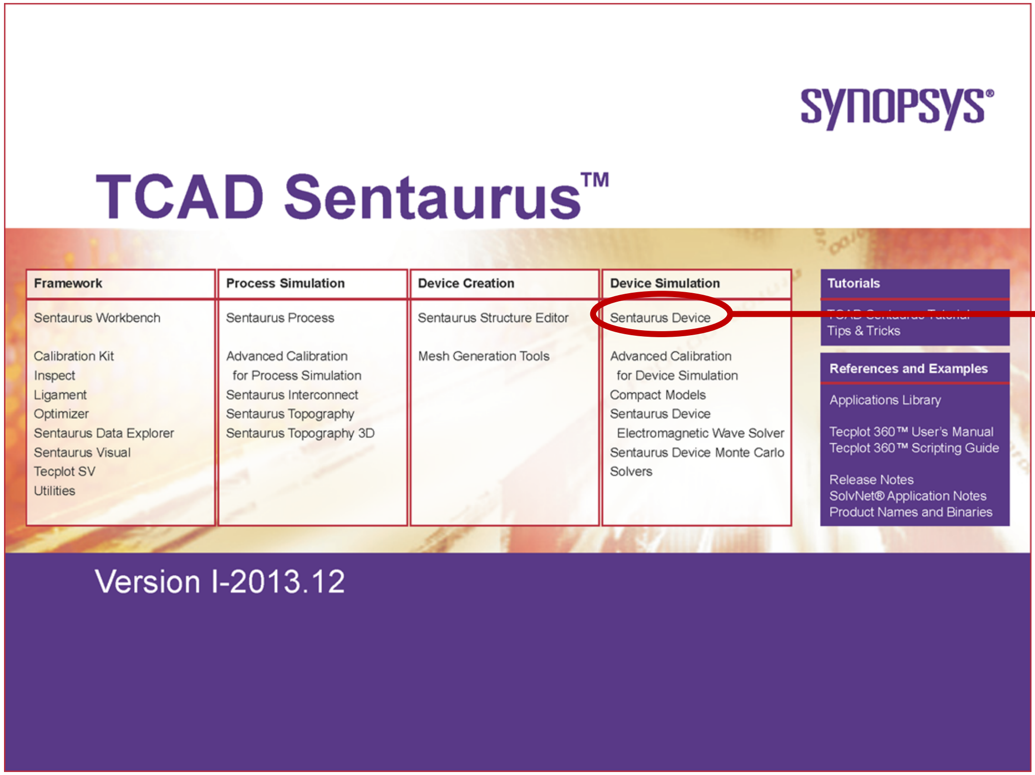
  n*nodenumber*.plt to visualize the device electrical characteristics

- The difficult part about Sdevice is not programming in itself but understanding the simplification inherent to the chosen physical models !
- It is in general not trivial to understand which physical models must be included
- Also the choice of material parameters and of the numerical parameters can be challenging

File naming conventions of SDE and Sdevice tools



The manuals: where is the description of the device physics?



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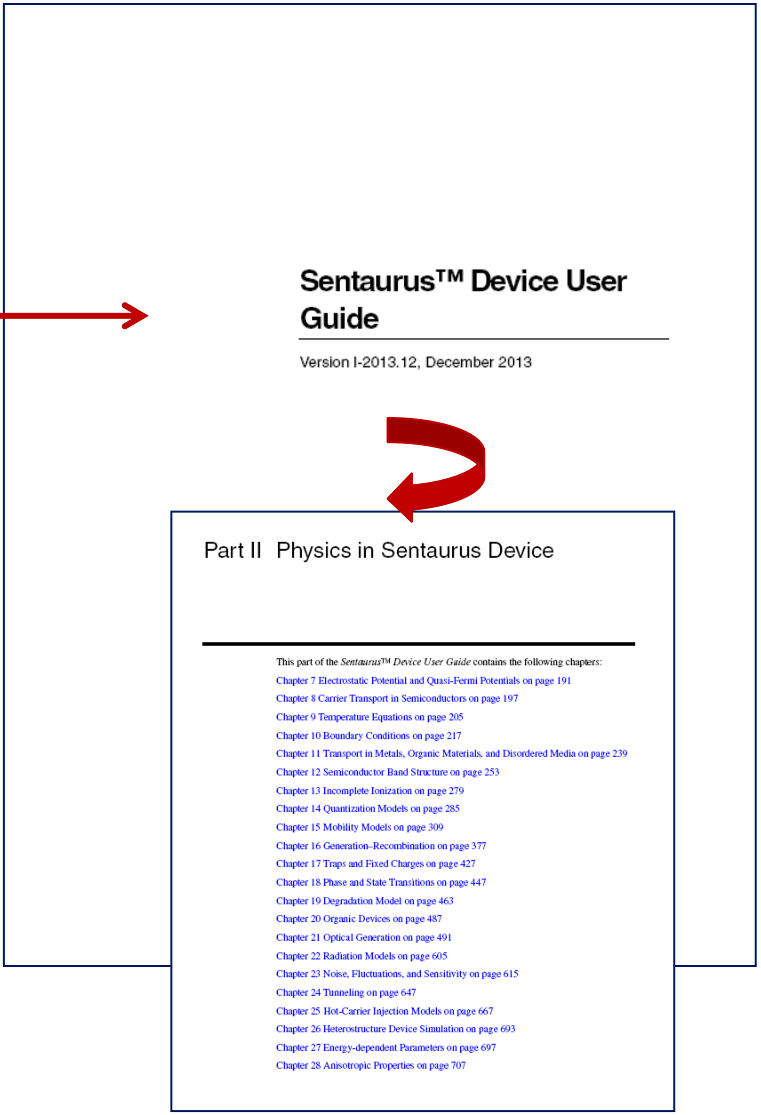

Sentaurus™ Device User Guide

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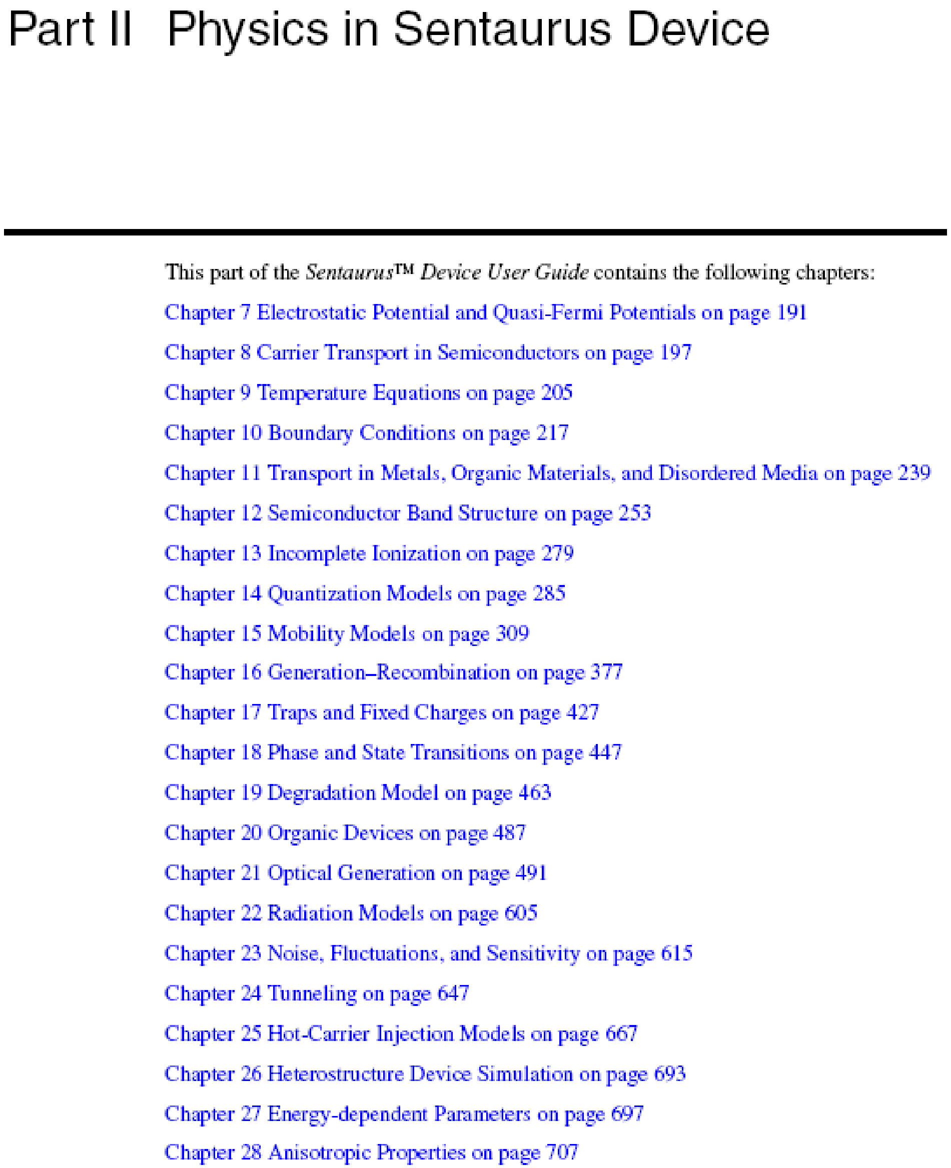
Part II Physics in Sentaurus Device

This part of the *Sentaurus™ Device User Guide* contains the following chapters:

Physics in Sentaurus Device



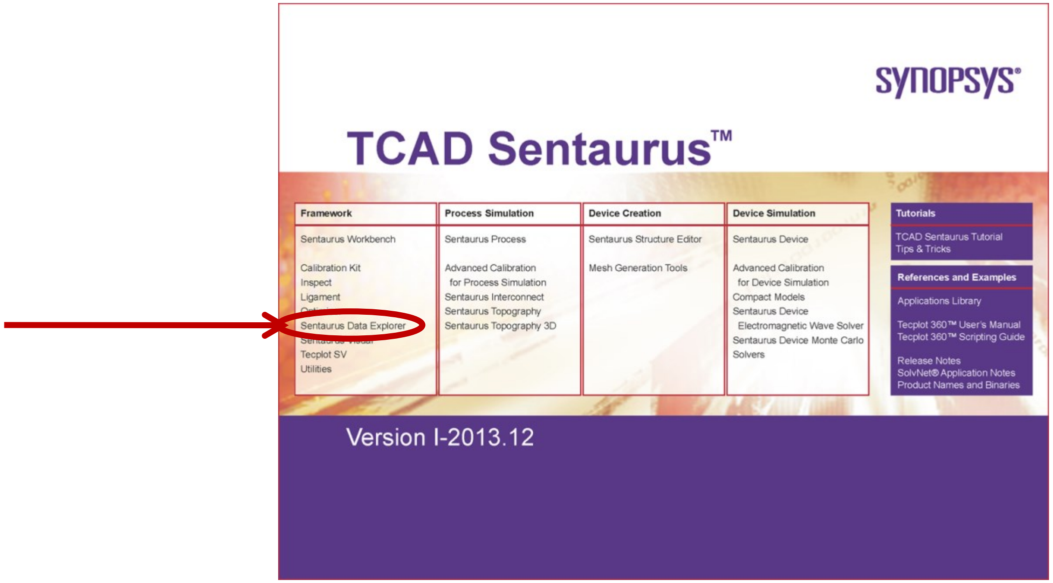
Part II Physics in Sentaurus Device

This part of the *Sentaurus™ Device User Guide* contains the following chapters:

Additional tools (1) : Tcl

- **Tool Command Language (Tcl)**
  - Commands in Tcl can be inserted in the command files of the Synopsys Sentaurus Tool
  - Tcl allows increased flexibility, providing the means of adding:
    - **Conditional statements (control structures)**
    - **Automation of export and manipulation of computed quantities**

- More information about Tcl can be found in the Sdevice manual and in the Sentaurus Data Explorer manual of Sentaurus Synopsys manual's suite



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Additional tools (2) : PMI (1)

- The **PMI (Physical Modeling Interfaces)** is an advanced additional tool provided in Sentaurus Sdevice to increase the flexibility of the software.
- **The PMI allows user to add its own physical models to express many physical properties.**

- <u>Example.</u>
- Heat equation: $-\nabla \cdot k\nabla T = Qj$

  where k is the thermal conductivity, T is the temperature and Q_j is the Joule heating generation term (given by the scalar product of current density and electric field)

- Heat equation cannot be modified, but the user can provide its own expression for k as a function of other predefined physical quantities.
- User functions (libraries) are written in *C*++
- Libraries must be compiled and then are loaded at run-time.

Additional tools (2) : PMI (2)

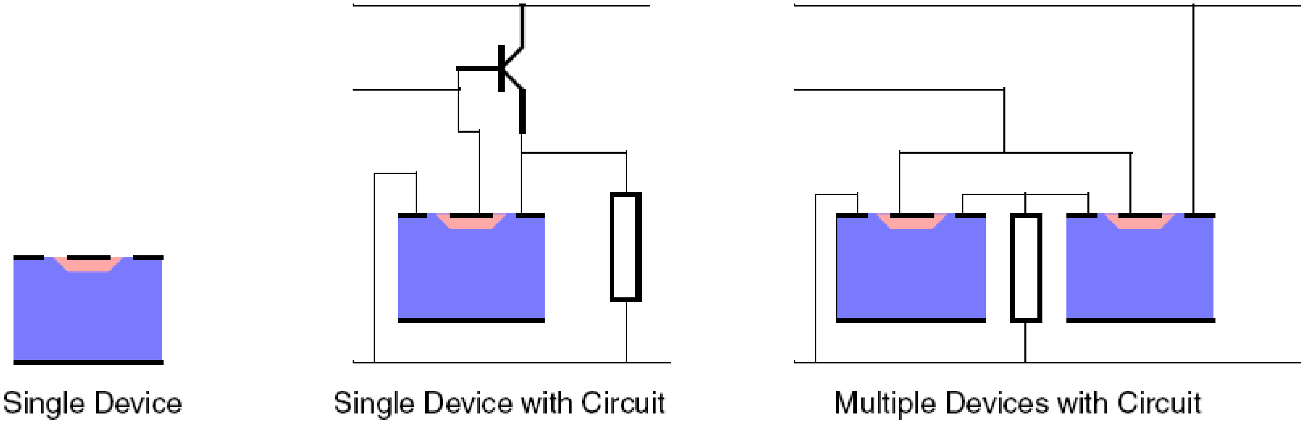
- Accessible models:
  - Generation–recombination rates / Lifetime
  - Avalanche generation, i.e. ionization coefficient
  - Band gap, Band-gap narrowing, Electron affinity
  - Effective mass
  - Energy relaxation times
  - Thermal conductivity, Heat capacity
  - Optical absorption, Refractive index
  - Metal Resistivity
  - Mobility
  - … and many others

Additional tools (2) : PMI (3)

- Physics
  - Formulate the analytical expression of the model
  - Compute the derivatives with respect to relevant input variables
- Coding
  - Implement C++ model and derivatives in `modelname.cc`
  - Compile run-time object using `cmi`
  - Resulting `modelname.so.arch` is architecture dependent
- Execution
  - Introduce the PMI path in the Sdevice `File{ }` section
  - Specify model name in `Physics{modelname}` section
  - The PMI model parameters accessible from Sdevice parameter file as : `modelname{}`

Mixed-mode simulations

- A *mixed-mode* simulation is available, meaning that in Synopsys Sentaurus it is possible to **simulate a circuit in which a device is inserted.**
- The mixed device and circuit capabilities give Sentaurus Device the ability to solve three basic types of simulation: single device, single device with a circuit netlist, and multiple devices with a circuit netlist



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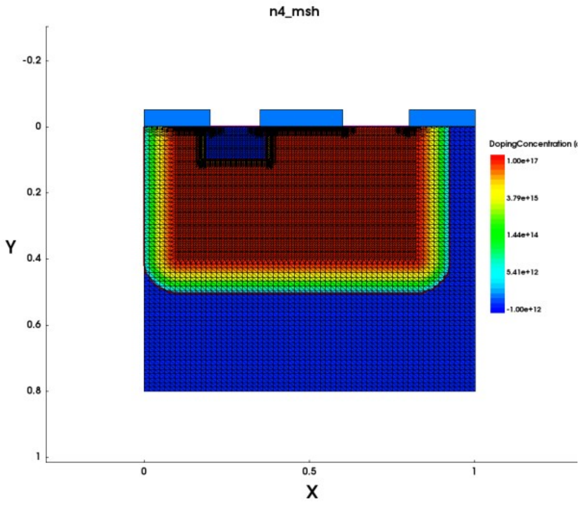
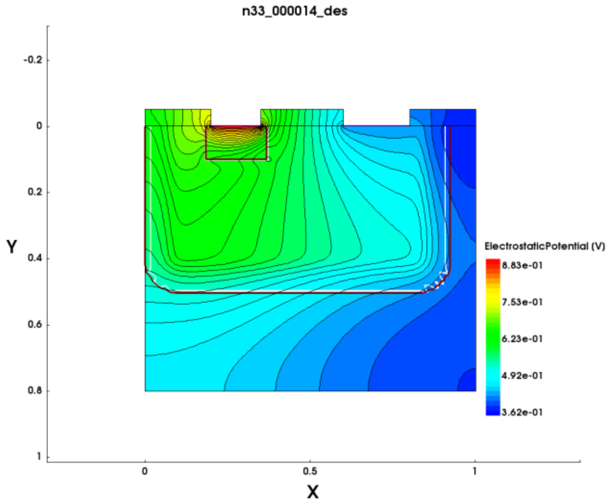
Examples of simulation output

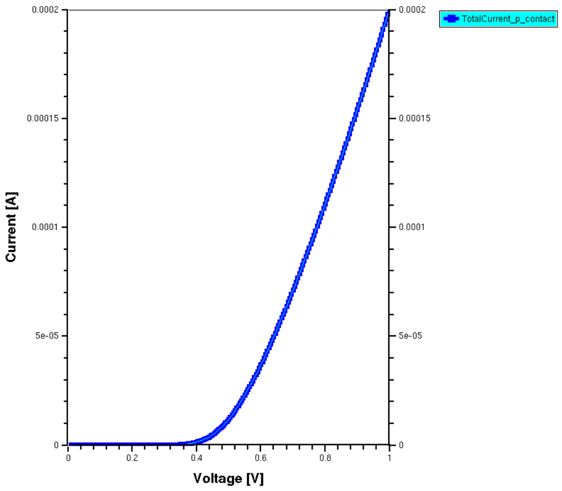
- `.tdr` files must be opened with Sentaurus Visual (Svisual)
- `.plt` files must be opened with Inspect



output of SDE simulation: geometry, mesh and doping concentration (displayed with Svisual)



output of Sdevice simulation: electrostatic potential (displayed with Svisual)



output of Sdevice: IV characteristics of a pn diode in forward bias (displayed with Inspect)

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Conclusions (1)

- Synopsys Sentaurus TCAD is the most developed software package for TCAD simulations, in fact it is the **industry-standard**
- It is a **software suite**, that is it contains several dedicated tools, each of them having its own programming language
- Among the tools, the **Sentaurus Workbench is the gateway that enables the control of all the simulation flow**

Conclusions (2)

- Flow of a DEVICE TCAD simulation:
  - creation of a geometry and of the numerical mesh

    creating a numerical mesh for convergence cannot be trivial, frequently involving a trial-and-error procedure (trade-off between convergence/accuracy and simulation time)

  - choice of the physical models to be solved, of boundary conditions and material parameters

    which are the approximation inherent in the applied models?

    Are they acceptable? Should we include additional physics?

  - tweak of numerical parameters to assure convergence of numerical solution

    as for numerical mesh, mainly based on trial and error/experience

  - understands the output of the simulation

    Which is, in essence, the results of the simulation? How things can be changed for better performance/ to obtained the desired results?